ARM TR-041

Solar Radiance Transmission Interferometer (SORTI) Handbook

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1. General Overview

The Solar Radiance Transmission Interferometer (SORTI) is a ground-based optical radiometer that produces ultra-high resolution infrared spectra of solar radiation transmitted through the atmosphere. The ultra-high spectral resolution of this instrument permits verification of theoretical line-by-line (LBL) calculations of atmospheric transmittance. The spectra produced may be used to quantify the total integrated columnar amounts of N_2O, O_3, NH_3, and HNO_3 in the atmosphere.

2. Contacts

2.1 Mentor

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2.2 Instrument Developer

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Frank Murrcray: 303-871-3557 at University of Denver, Instrument Designer

3. Deployment Locations and History

The SORTI instrument is located in the Optical Trailer at the Southern Great Plains (SGP) site (Oklahoma). The optical trailer is located on the ground at an altitude of 315.2 meters.

4. Near-Real-Time Data Plots

This section is not applicable to this instrument.

5. Data Description and Examples

A portion of the data taken by SORTI on January 9, 1995, at 2:00 pm central time is available in Figure 1. The image below (Figure 2) is taken from reference 3 and shows the calculated ozone concentration above Mauna Loa, Hawaii. The cross data points are from Dobson calculation, and the squares are values derived from fourier transform infrared radiometer (FTIR) instrumentation with methods similar to methods to be employed for column amounts at the SGP site. The FTIR-derived values were multiplied by 1.046 to compensate for a 4.6% low prediction of Ozone (using Dobson values as reference).

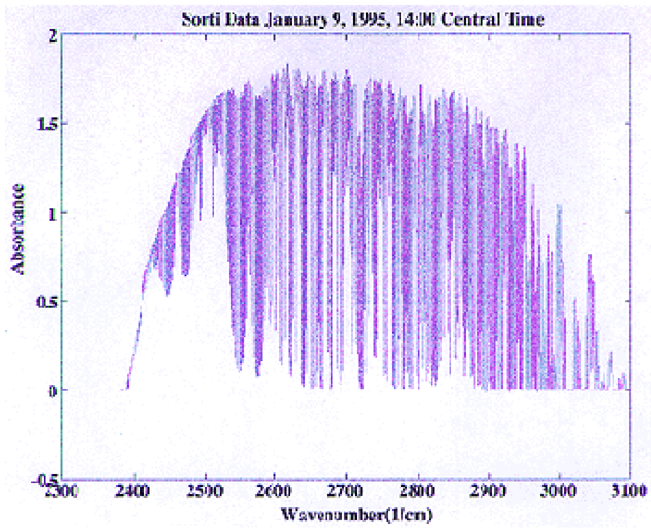

Figure 1.

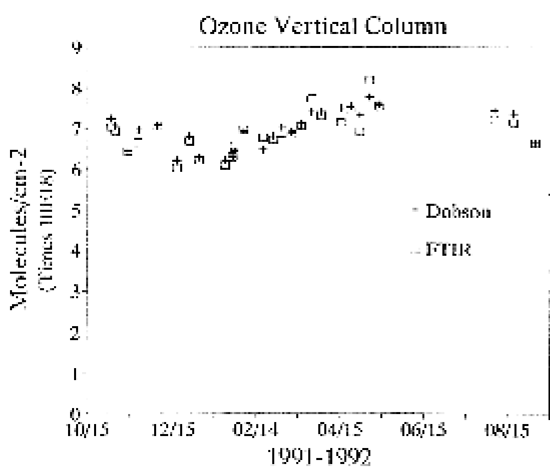

Fig. 2. Total column ozone measured by the FTIR and Dobson techniques, after multiplying the FTIR values by 1.046.

Figure 2.

5.1 Data File Contents

5.1.1 Primary Variables and Expected Uncertainty

Column amounts of N_2O, HNO_3, O_3, and NH_3 are all measured with the SORTI instrument.

5.1.1.1 Definition of Uncertainty

The Ozone column concentration is compared with known values using Dobson values as reference values in reference 3; agreement is within 5% during the entire 10-month period.

Comparisons done with N_2O in the past have shown agreement within 10% (Frank Murrcray, private communication). Uncertainties in the other three species: NH_3, and HNO_3 are expected to be within 10% by analogy with the N_2O method.

5.1.2 Secondary/Underlying Variables

This section is not applicable to this instrument.

5.1.3 Diagnostic Variables

This section is not applicable to this instrument.

5.1.4 Data Quality Flags

A data ingest has not been written at this time. Plans are under way to have an ingest procedure to place the files into netCDF format.

5.1.5 Dimension Variables

This section is not applicable to this instrument.

5.2 Annotated Examples

This section is not applicable to this instrument.

5.3 User Notes and Known Problems

This section is not applicable to this instrument.

5.4 Frequently Asked Questions

Are data taken continuously?

No, data are currently taken three times a day: When the sun is at a 30-degree elevation in the morning, once at high noon, and finally when the sun is again at a 30-degree elevation in the afternoon.

Are data taken at night or on cloudy days?

No, data are taken only during clear-sky days when the sun reaches the three elevations described above.

Are independently acquired data on column amounts available for any of the species? If so, from what source?

Ozone sondes are not available for comparison. However, as discussed in reference number 3, the FTIR-derived ozone column amounts compare favorably with those derived from Dobson techniques (ultra violet).

Are there any other references you can recommend?

Reference number 4, although it discusses the measurement of ethylene, the algorithms and techniques are very similar to those used to derive column concentrations of all of the species, answers this question.

Ozone soundings were made during the ARM Enhanced Shortwave Experiment (ARESE). Was the SORTI running then?

Yes, SORTI was running well during the last week of ARESE and gathered useful data. If the Ozone sounding results are made available to Tom Stephens of the University of Denver, then he can provide SORTI - ozone sounding comparisons within one week.

6. Data Quality

6.1 Data Quality Health and Status

The following links go to current data quality health and status results:

- DQ HandS (Data Quality Health and Status)
- NCVweb for interactive data plotting using.

The tables and graphs shown contain the techniques used by the Atmospheric Radiation Measurement (ARM) Program's data quality analysts, instrument mentors, and site scientists to monitor and diagnose data quality.

6.2 Data Reviews by Instrument Mentor

As noted in the notes on the absolute solar transmittance interferometer (ASTI), automated data quality products have not yet been developed for the SORTI. The SORTI provides data uncalibrated in terms of radiance units. Instrument mentor Connor Flynn plans to examine SORTI data by comparison to ASTI data in the spectral range 1950-4300 cm^-1, where the spectral regions overlap for the two systems. The ASTI will thus act as a calibration transfer standard for the SORTI. Because the SORTI has better spectral resolution than the ASTI, comparison of the two sources of data requires that the SORTI data be effectively de-resolved, either by manipulation of the spectra or the native interferograms. Then interpolation can be used to infer the calibration coefficients for the original, high-resolution SORTI spectra. The effects of differing fields of view and scan times for the SORTI and ASTI need to be addressed.

> One of the data products that will be developed is a reduced spectrum from the SORTI for applications not requiring data with the high resolution of 0.0035 cm^-1. A QME will be proposed to compare the reduced SORTI data set in suitable spectral regions with data from the rotating shadowband spectroradiometer (RSS) and possibly the shortwave spectroradiometer (SWS) if it was modified in the future to detect direct-beam irradiance. Automatically generated graphical displays of the summary spectra are desired.

The overlap spectral regions listed above for the SORTI and ASTI do not include the SORTI bandpass filter region (620-1350 cm^-1) used for retrievals of column amounts. These column amount retrievals do not require spectra with absolute calibration. Code developed at the University of Denver runs in an automated manner to produce the column retrievals. This code should be moved to the SGP site data system, where data quality checks could be implemented.

6.3 Data Assessments by Site Scientist/Data Quality Office

All Data Quality Office and most Site Scientist techniques for checking have been incorporated within DQ HandS and can be viewed there.

6.4 Value-Added Procedures and Quality Measurement Experiments

Many of the scientific needs of the ARM Program are met through the analysis and processing of existing data products into "value-added" products or VAPs. Despite extensive instrumentation deployed at the ARM sites, there will always be quantities of interest that are either impractical or impossible to measure directly or routinely. Physical models using ARM instrument data as inputs are implemented as VAPs and can help fill some of the unmet measurement needs of the program. Conversely, ARM produces some VAPs not to fill unmet measurement needs, but to improve the quality of existing measurements. In addition, when more than one measurement is available, ARM also produces "best estimate" VAPs. A special class of VAP, called a Quality Measurement Experiment (QME), does not output geophysical parameters of scientific interest. Rather, a QME adds value to the input datastreams by providing for continuous assessment of the quality of the input data based on internal consistency checks, comparisons between independent similar measurements, or comparisons between measurement with modeled results, and so forth. For more information, see VAPs and QMEs web page.

Column amounts of N_2O, HNO_3, NH_3, and O_3 will be available. A VAP comparison with lbl models is in the planning stage for the SORTI. A line-shape QME comparison with spectral lines (currently used in LBL models) may also be developed.

7. Instrument Details

7.1 Detailed Description

7.1.1 List of Components

The SORTI (schematic) is composed of the following parts:

- Bruker model 120M-high resolution FTIR
- Solar tracker (built at the University of Denver) (see Figure 3)
- Two infrared detectors (used in the FTIR instrument): HgCdTe and InSb (both manufactured by EG&G Judson)
- Solar tracker position sensitive detector (made by Silicon Devices Incorporated)
- Bandpass filters (manufactured by North Umberland Optical Co., England)
- Filter wheel attachment (manufactured by Bruker)
- Data acquisition system (comprises a Pentium PC compatible machine running Bruker's "Opus 2.2" software in the OS2-Warp platform).

Solar tracker (built at the University of Denver)

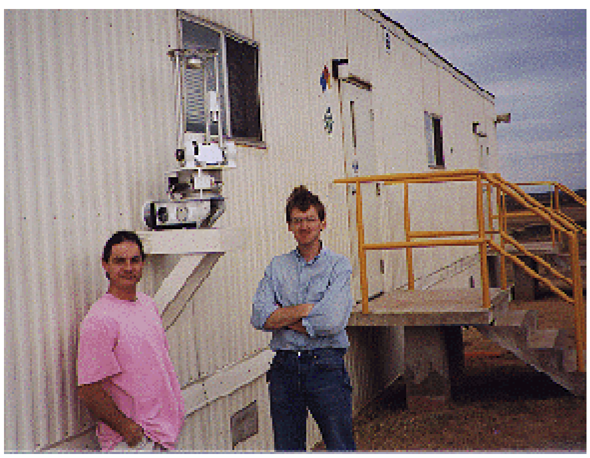

Figure 3.

7.1.2 System Configuration and Measurement Methods

The SORTI instrument is located in the Optical Trailer at the SGP (Oklahoma) site. The optical trailer is located on the ground at an altitude of 315.2 meters. A solar tracker mounted on top of the instrument trailer receives and directs the solar radiation into the interferometer through a hole cut in the south wall of the trailer. Spectra are collected three times per day on clear-sky days; once in the morning, once at zenith, and once in the afternoon. The measurements in the morning and afternoon are taken when the sun reaches a 30-degree elevation with respect to the horizon. Two spectra are coadded to increase the signal-to-noise ratio. The approximate time to gather the two spectra to be coadded over all six spectral ranges is 5 minutes.

The solar tracker, visible in the attached photograph, consists of a position-sensitive detector with a neutral density filter placed in front. The position of the sun is determined by the position-sensitive detector, the two servo motors: azimuth and elevation then rotate the collection mirror to the location of the mirror based upon the output of the position-sensitive detector. The light from the collection mirror is then steered into the FTIR instrument with a series of relay mirrors.

Once the sun's energy is directed into the FTIR, the energy must pass through one of six filters as selected by the filter wheel. The filters are used to increase the signal to noise ratio. Recalling that detectivity goes as "one over" the square root of the bandwidth, it is advantageous to limit the bandwidth of the incident light. The broadband light exiting the filter is then passed through both legs of the Bruker interferometer and combined at the surface of the detector where an interferogram, I(x), is formed. The interferogram is then fourier transformed using a "fast fourier transform" into the more familiar Intensity as a function of frequency, I(v). The filter wheel is then rotated until all six spectral regions are collected.

7.1.3 Specifications

Bandpasses: 620 to 1350 1/cm, 1500 to 2050 1/cm, 2020 to 2550 1/cm, 2420 to 3080 1/cm, 3010 to 3830 1/cm, and 4020 to 4300 1/cm.

Spectral Resolution: 0.0035 wavenumbers (apodized).

Wavenumber Accuracy: 0.5 parts per million absolute, 0.05 parts per million relative.

Measurement Periods: The SORTI instrument makes measurements at all of the above wavenumber ranges three times per day. The first measurement occurs when the sun reaches an angle of 30 degrees with respect to the horizon. The second measurement period is at noon (maximum solar angle with respect to the horizon). The final measurement period occurs when the sun reaches a 30-degree angle again with respect to the horizon.

Length of time needed to collect spectra: Each spectra is a coadd of two spectra; the instrument takes about 5 minutes to collect the two coadded spectra in all of the wavelength ranges.

Atmospheric height sampling interval: The SORTI instrument uses the sun as its source of light and so its corresponding range would have to be listed as the top of the atmosphere. That is, the absorption observed is due to extinction, and scattering from the top of the atmosphere all of the way down to the ground level.

Field of View: The optical telescope has a 6 milliradian (.3-degree) field of view.

Temperature Range for operation: The optical bench was designed to operate in room temperature conditions. The tracker unit (outside) was designed to operate in the range of minus 20 centigrade to plus 40 centigrade.

Humidity Range: The optical bench is dessicated, operation in high humidity (greater than 40% RH) requires exchanging the dessicant more frequently or a dry nitrogen purge (not currently hooked up).

Wind Range for the Solar Tracker: The Solar Tracker was designed to operate in high winds (up to 40 knots). However, during windy periods dust may settle on the mirrors, requiring more frequent cleaning.

Power Requirements: 110 VAC times 5 amps of uninterruptible power (UPS), and 110VAC times 2 amps of non UPS power.

Mechanical Dimensions: 2 ft by 2 ft for the solar tracker (outside), and 3.5 ft by 8 ft inside the optical trailer.

Weight: Optical Bench: 1200 pounds, pump: 200 lbs.

7.2 Theory of Operation

The FTIR spectrometers measure light absorbed or emitted from a sample as a function of wavelength. They consist of an optical system for collecting light and concentrating it, an interferometer for algebraically combining the light from the two light paths, a detector to change the light intensity into an electrical signal, signal conditioning electronics, and a computer for extracting spectral data from the signal using FTIR methods.

In general, interferometers combine light from two light paths algebraically resulting in variations in light intensity across the aperture of the interferometer called interference fringes (for non-coincident or non-identical wavefronts). One light path is scanned to vary the optical pathlength. The other path is a reference path. Consider a Michelson interferometer looking at monochromatic light from a collimated expanded laser beam, in which the incident beam is split into two equal length paths by a beamsplitter. Also assume that each path ends in a plane front surface mirror, which is aligned such that the surfaces are normal to the beam, as shown in Figure 4.

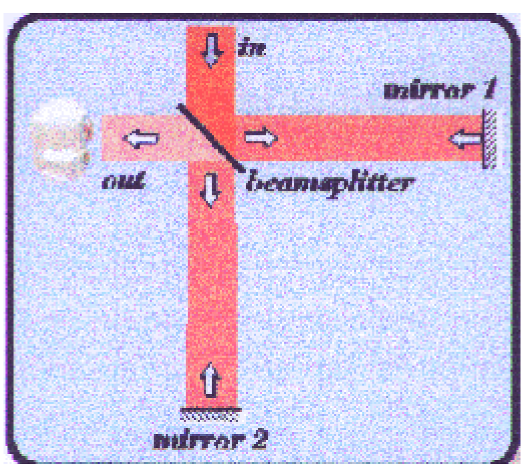

Figure 4.

If the mirrors are aligned exactly so that the distance traveled by light is point-for-point identical over the beam for the two paths, the observer will see a uniformly bright entrance aperture through the interferometer. If the paths differ by a half-wavelength, the observer will see a uniformly black aperture. For intermediate positions, the intensity will be proportional to the cosine of the phase angle (relative fraction of a half-wavelength path difference).

This observation is true only for monochromatic light. If a second monochromatic wavelength is added, the cross-section will have different intensity for each of the two wavelengths because the difference in pathlengths between the two paths will be a different multiple (or fraction) of wavelengths for each wavelength. For additional wavelengths, intensity contributions are algebraically summed.

If light entering the interferometer is an unknown combination of wavelengths, like light from a source having a broadband spectrum, the result will be a complex combination of intensities due to the multiple wavelengths. As the optical pathlength of one path is slowly, but uniformly changed, the difference in pathlength for each wavelength will change. Because the wavelengths are different, the path difference expressed as a factor of the wavelength will be different for each wavelength, and will change at a different rate. Path differences, resulting in a variation in output intensity, will change more quickly for short wavelengths than for long wavelengths. If a detector converts the intensity variations into electrical variations, temporal signal will be a superposition of cosines with periods representing the time variations in intensity. Analysis of this series into its component frequency components (with coefficients characteristic of the relative intensities of the individual wavelength components present in the incident light) is accomplished using a FTIR algorithm. The algorithm is ideally suited to breaking down signals comprising a series of sines or cosines, resulting in the electromagnetic spectrum of the incident light.

The function of the Helium Neon laser in a modern FTIR is often misunderstood. Its sole purpose is to measure the position(x) of the moving mirror, the so called retardation distance. The helium neon laser is used in a separate interferometer, called the reference interferometer, which shares the moving mirror with the infrared interferometer. In this way, fringes are counted in the reference interferometer, which allows a precise measurement of the retardation position, x. With the interferrogram, I(x), from the infrared interferometer, and the retardation position, x, the spectra can be obtained by a fast fourier transform.

Column amounts of N_2O, O_3, NH_3, and HNO_3 are obtained by least squares fitting with known spectral features of these four molecules and the specrta of water. To determine the N_2O and O_3 column amounts, the spectral region between 1161 and 1163 wavenumbers is used. In this spectral region, three lines are due to O_3 and one is due to N_2O. The amounts of O_3 and N_2O are varied until the residual error, the difference between observed and simulated spectra, is minimized. Similarly, the region between 867 and 869 wavenumbers is used to determine the concentration of NH_3, and HNO_3. Water vapor is also used as a pure component spectra in the least squares routine, but the column amount of water vapor is not reported due to the variable nature of this quantity near the ground.

More formally, the optical path of the light through the atmosphere is calculated with FASCODE. The spectral features then are fit with the program SFIT1.09d. SFIT is a least squares line analysis package that draws upon the HITRAN database, draws upon accepted molecular VMR profiles, and uses the sonde data from the SGP site. This type of analysis is well established and works with relative data (as well as absolute data). Currently, this analysis is conducted at the University of Denver. There are plans to automate the process and move the analysis to the SGP site.

7.3 Calibration

7.3.1 Theory

Measurements of the solar radiance at four or five different zenith angles will produce spectra of different amplitudes. Langley regressions will be done when operation of the instrument allows for the acquisition of more low-zenith-angle spectra. When the Langley regressions are complete, comparisons to top-of-the-atmosphere radiance (satellite data) can be made. Because the instrument is using the solar photosphere (6000K) as a source, calibration sources are difficult to obtain. Wavelength registration problems are uncommon in FTIR instruments because they count fringes in the reference interferometer using the known wavelength of a Helium-Neon laser.

7.3.2 Procedures

This section is not applicable to this instrument.

7.3.3 History

Column amounts will be available by the end of August 1996. At that time, comparisons with ozone column amounts derived from Dobson't method will be used. The background concentration of N_2O is fixed at around 310 parts per billion and will be used as a quality check.

7.4 Operation and Maintenance

7.4.1 User Manual

This section is not applicable to this instrument.

7.4.2 Routine and Corrective Maintenance Documentation

This section is not applicable to this instrument.

7.4.3 Software Documentation

This section is not applicable to this instrument.

7.4.4 Additional Documentation

See the Preventative Maintenance Procedure Summaries for the SORTI at the SGP site.

Daily operation of the SORTI requires that the solar tracker cover be removed and replaced at the end of the clear-sky day. This practice minimizes the exposure of the solar tracker to dust and precipitation. Currently, maintenance is performed every six months by Tom Stephens of the University of Denver.

The optics in the solar tracker and FTIR are cleaned, the drive mechanisms are lubricated, and the dessicant inside the FTIR is removed. During the rainy season (spring in particular), the dessicant is replaced every two weeks.

A. Calibrations and Related Performance Checks

1. What are factory-recommended calibration procedures?
   Not absolutely calibrated; NIST traceability does not apply.

2. What are the factory-recommended performance checks?
   Standard Bruker Acceptance tests on spectrometer - in Ops manual.

3. What are the mentor calibration procedures?
   A comparison of absorption lines with known standards. Periodic determinations of standard gases for quantification checks.

4. What are the mentor performance checks?
   A comparison of wavelengths, absorption strengths, and spectral intensity to reference spectra.

5. How are calibration and related performance checks documented?
   In daily instrument logs.
   a. Where are procedures documented? In the Site Ops manual.
   b. Have major changes to calibration procedures occurred? No
   c. Are major changes to calibration procedures expected to occur? No

6. Who implements calibration and performance checks?
   Mentor calibration and performance checks are initiated by Site Ops, CPU operation (automatic), and Associate Scientist.

7. What is standard schedule of calibrations and checks?
   A series of daily checks are incorporated in QC/QA plan. Additional tests are conducted as necessary on a periodic basis.

8. How are the calibration and check procedures initiated (queued)?
   a. Scheduled Calendar Event: Associate Scientist.
   b. Data Inspection: Automated data inspection.
   c. Instrument Failure: Yes.

9. How long does it take to perform calibration and performance check procedures?
   An automated test is completed prior to ingest - takes less than one hour.

10. Are any data affected or lost during calibration or performance check procedures?
    No, spectra not passing QC/QA are documented and removed from ingest.

11. What are corrective procedures when calibrations and or performance checks fall behind schedule?
    Calibrations and performance checks are done concurrently. Scheduled tasks will only fall behind in case of instrument failure. Cannot recover missed data on failure.

B. Calibration Data:

1. Where are calibration data documented?
   All calibration, QC and QA checks, will be documented in the Site Ops Manual - hardcopy. Instrument mentor will provide site with hard copy and electronic copy. Site will have permission to disseminate in any media with prior approval.

2. Where are calibration coefficients and algorithms applied to convert data to geophysical units?
   Calibration procedures will be on front-end CPU with electronic copy of coefficients.

C. Maintenance Procedures:

1. What are the factory-recommended maintenance procedures (preventive and corrective)?
   Maintenance procedures are rather lengthy. Complete documentation will be provided with Site Ops manual.

2. What are the mentor preventative and corrective maintenance procedures?
   Maintenance procedures are rather lengthy. Complete documentation will be provided with Site Ops manual.

3. How are maintenance procedures documented?
   a. Where are procedures documented? In Site Ops Manual
   b. Have major changes to maintenance procedures occurred? No
   c. Are major changes to maintenance procedures expected to occur? No

4. What is the procedure schedule?
   A series of daily PM1s are incorporated in QC/QA plan. Additional tests as necessary on periodic basis.

5. How are the procedures initiated (queued)?
   a. Scheduled Calendar Event: yes
   b. Work Order: yes
   c. Data Inspection: yes
   d. Instrument Failure: yes
   e. CPU automated tasks: yes.

6. How long does it take to perform maintenance procedure?
   Regular PM tasks are transparent to the system and are performed continuously. Corrective maintenance tasks can take from five minutes to a month depending on the problem.

7. Are any data affected or lost during maintenance procedure?
   No data are lost during PM tasks. Data may be lost during CM tasks.

8. How are potential affects to data documented?
   In instrument log - general terms in Site Ops Manual.

9. What are corrective procedures when maintenance falls behind schedule?
   Find someone to perform maintenance and discuss reassigning work loads.

10. Where is actual maintenance work documented?
    Instrument logs and site logs.

D. Data Integrity and Quality Inspections:

1. What nodes or activities along the data pipeline affect (or can potentially affect) the data stream?
   a. Controller Boxes: yes
   b. Microprocessors: yes
   c. Data Logger: no
   d. Communication lines/links: yes
   e. Calibration Data files: no
   f. Ingest Modules: yes--Disk space limited (1Gb or one to two months data).

2. What are current difficulties?
   Work on ingest module and the site data system (SDS) has not been started nor have we been informed as to when it will start.

3. List and describe any standard or non-standard data inspections (active or planned) under each of the following categories:
   a. Data Existence check: yes
   b. Mentor QC checks (during ingest): instrument function, weather, and data quality.
   c. Mentor QC checks (outside of ingest): data product quality by comparison with known line shapes, intensity of N2O peak (relatively fixed at 300 ppb times path).
   d. Within Platform Check: every minute
   e. Multiple Platform Check: NA
   f. QMEs/VAPs: No QME planned at this time
   g. Other automated netCDF file checks: No netCDF ingest available yet
   h. Other analytic tools or algorithms: Low-quality data will be spotted when column amounts do not make physical sense. The instrument mentor at PNNL may write an automated QME to make sure column amounts fall within a physical range.

4. Does storage media exist on the instrument system to back up data and store it for delayed data ingest?
   Storage exists in form of 1 Gb hard disk. This is sufficient to store two weeks to two months of data (depending on number of clear sky days).

7.5 Glossary

Column Amount - Integral amount of species existing in a column from ground to the top of the atmosphere. Column amount says nothing of the profile.

LBL Model - The most detailed model of atmospheric radiation and absorption. The radiance is calculated one spectral line at a time.

NetCDF - A standard data format developed by the National Center for Atmospheric Research (NCAR) and Unidata.

7.6 Acronyms

ARESE	Atmospheric Research and Modeling Extended Shortwave Experiment.
ASTI	absolute solar transmittance interferometer
FTIR	fourier transform infrared radiometer
I_o	Intensity of beam with no absorbance along path length
IRF	Instaneous Radiant Flux
LBL	line-by-line
NCAR	National Center for Atmospheric Research
PNNL	Pacific Northwest National Laboratory
Ppb	parts per billion
QA	quality assurance
QC	quality control
QME	Quality Measurement Experiment
RSS	rotating shadowbank spectroradiometer
SDS	site data system
SORTI	Solar Radiance Transmission Interferometer
UPS	uninterruptible power
VAP	value-added product

7.7 Citable References

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